

Molecular Motors and Microtubules: Patterns and Self-Assembly

Scientific Achievement

Researchers at Argonne National Laboratory and University of California at San Diego have developed a new multi-scale approach to elucidate the self-assembly of biological microtubules and molecular motors into ordered coherent structures such as asters, vortices and bundles. Using the analogy between the celebrated Maxwell Model for inelastistic colliding particles and interacting microtubules, a theory which illuminates the dynamics of the local concentration and orientation of rod-shaped objects was derived from elementary interaction rules. At a large enough mean density of rods and concentration of molecular motors, the model naturally describes the orientation instability which ultimately leads to the formation of coherent structures. This approach can be used as a foundation for constructing a multi-scale model of self-assembly for microtubules and molecular motors.

One of the most important functions of molecular motors is to organize a network of long filaments (microtubules) during cell division to form cytoskeletons of daughter cells. A dividing cell has to spatially separate its newly duplicated chromosomes. To do so, it uses a bipolar spindle, a complex molecular structure made of many different protein components to accomplish this task with high precision. A series of in-vitro experiments focused on understanding the fundamentals of microtubule and motor self-assembly was pioneered in the group of Prof. Leibler at Princeton University. Depending on the motor concentration, the experiments revealed a rich variety of self-assembled static and dynamic patterns: star-like structures (asters), rotating vortices as well as long bundles of microtubules. Our theory, having no fitting parameters and derived from microscopic rules, gives a comprehensive explanation of their observed behavior and leads to testable predictions.

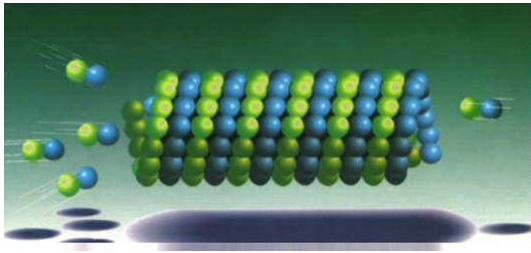
Significance

The understanding of the remarkably rich and intriguing self-organized behaviors found in simplified biological systems represents a significant breakthrough in our understanding of the physics of self-assembly of complex systems. Our results, based on the systematic derivation of a macroscopic continuum equation from microscopic interaction rules, constitute a totally new multi-scale approach to investigate self-assembly in biological systems in particular, and in complex nonequilibrium systems in general. The results, published in *Phys Rev E* **71**, 050901 (2005), stimulated further experiments in bio-inspired self-assembly in complex systems with possible applications for nanotechnology. Our theory was presented at more than 10 invited talks, including the American Physical Society March Meeting 2006. It generated a new seed proposal on multiscale modeling of microtubules' self-organization with DOE-MICS which was funded in 2006.

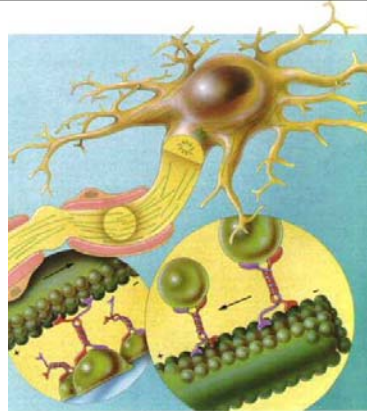
Performers

Igor Aronson (ANL-MSD); Lev Tsimring (University of California, San Diego)

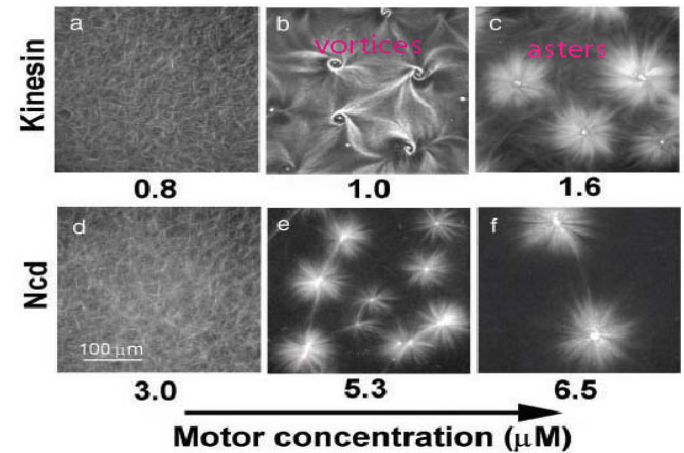
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Microtubules: stiff hollow chiral nano-rods
•Length up to 20 μm , diameter 24 nm



Molecular motors and microtubules in neurons



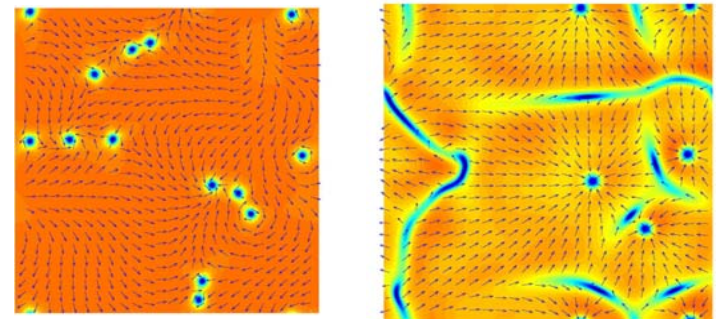
Asters and vortices in in-vitro experiments with microtubules and motors, group of Stanislav Leibler, Princeton University

Model:

- Stochastic master equation for tubules orientation
- Coarse-grained equations for density and orientation of tubules derived from master equations
- Solutions to coarse-grained equations exhibit asters and vortices

Future directions:

- Derivation of full three-dimensional model from realistic interaction rules
- Validation of interaction rules by the molecular dynamics simulations
- Extension of multiscale approach to new types of biological and biomolecular systems



Vortices (left) and asters (right) obtained by computer modeling

I.S. Aranson and L.S. Tsimring, *Pattern formation of microtubules and motors*, Phys. Rev. E 71, 050901 (2005)